Monte Carlo Simulation of Microelectronics for 3D Chemical Imaging

Modern microelectronic devices consist of complex three dimensional arrangements of different chemical phases such as silicon, silicon dioxide, metal such as copper and tungsten, and other compounds (e.g., diffusion barriers). The performance of these devices depends critically on their structure and fabrication precision. To better understand how to measure the three-dimensional chemical heterogeneity of microelectronic devices with nanometer spatial resolution, it is necessary to synthesize experimental data from the instruments used to characterize real devices. In analogy to multi-modal medical imaging techniques, the use of "phantoms" (synthetic samples) with exactly known properties is a powerful technique for improving the measurement infrastructure upon which all semiconductor manufacturers currently depend.

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Scanning electron microscopy (SEM) and analytical electron microscopy (AEM) can provide the analyst with huge amounts of detailed chemical data when used to characterize microelectronic devices. In many cases the datasets contains tens or hundreds of megabytes of spectral measurements which potentially contain the solution to performance problems. The challenge is to make sense of all these data and transform spectral curves into solutions to device problems. Understanding how known sample geometry produces complex spectral datasets is an important early step towards robust measurement methods that take advantage of the current generation of commercial analytical instrumentation. Both the manufacturers of the analytical instruments (microscopes and spectrometers) and the microelectronics industry (end users) are struggling to develop analysis strategies and algorithms to tame the flood of data provided by these new tools. NIST's strong background in measurement science, spectrum imaging methods, and multivariate statistical analysis place us in an unusually strong position to contribute a solution soon, to meet the immediate need faced by device fabricators as they introduce new processes and scale down existing device dimensions.

Based on a new set of Java classes written to function as a Monte Carlo engine for microanalysis simulations with complex sample geometries, the NIST researchers wrote a series of scripts to simulate phantom datasets relevant to microelectronics fabrication. Previously, such simulations could only predict simple (unrealistic) geometries insufficiently complex to model actual devices.

Fig 1 (a) 0° tilt perspective view of AEM cylinder phantoms (600 nm diameter by 1 μm long), blue arrow points to x-ray energy dispersive spectroscopy (XEDS) detector (b) same phantoms as seen by XEDS detector (c) view along tilt axis (d) 300 keV Monte Carlo electron trajectories, 100 electrons displayed at 1 of 32 horizontal beam raster locations. Figs 2 and 3 are the same as Fig 1 but sample tilted to 30° and 108°, respectively.

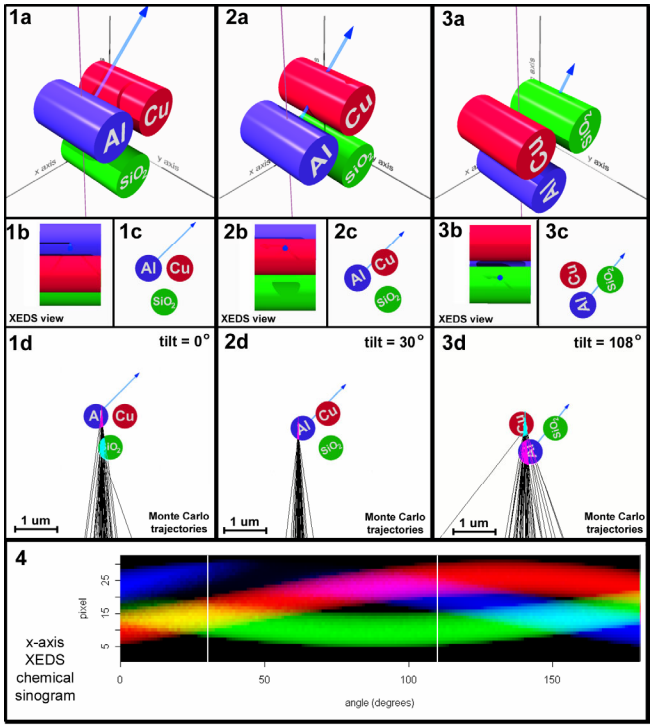

Fig. 4. "Chemical sinogram" displaying XEDS line intensities vs. sample tilt angle (horizontal axis) and x-axis beam raster position (vertical axis). Red is Cu Kα, green is O Kα, and blue is Al Kα. The vertical white lines denote 30° and 108°. Note attenuation of Al Kα by Cu cylinder near 30° tilt.

Untangling the self-absorption issues of x-rays and the internal electron scattering and transport phenomena for real device configurations has shed new light on spectrum image datasets used by analytical laboratories all over the world.

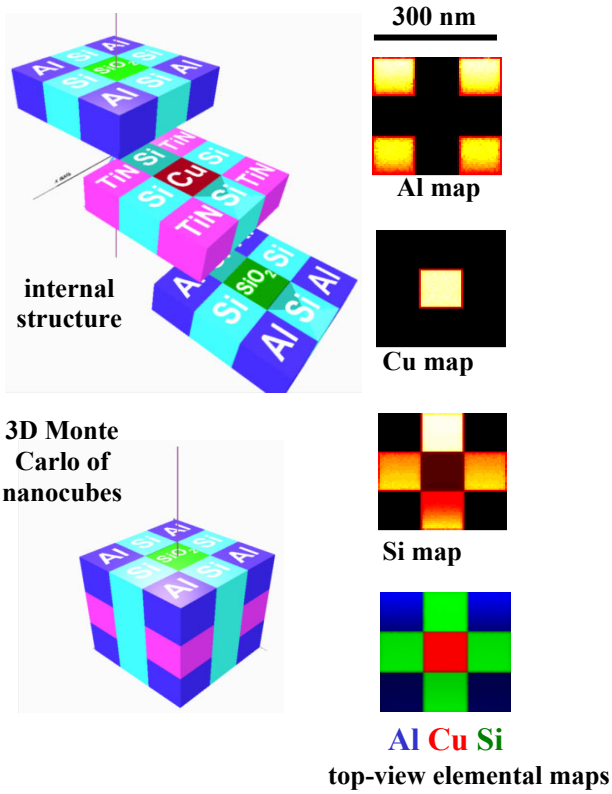

Fig. 5 A three-dimensional phantom sample containing aluminum, silicon, silicon dioxide, titanium nitride, and copper – all materials widely used in manufacturing semiconductor electronic devices. The "Rubik's cube" sample has been artificially sliced and the layers displaced for easier viewing of the interior chemical heterogeneity. In addition to the exploded view of the "Rubik's cube", here the assembled cube is seen as-simulated. On the right are four elemental maps generated from full x-ray spectrum image datatsets simulated using Monte Carlo techniques. The maps show the detected x-ray intensities for characteristic x-ray lines corresponding to aluminum, copper, and silicon. A three-color overlay is shown at the bottom.

Future Plans: This activity is just beginning and will play an important role in the remaining years of a NIST-wide Competence Project on 3D Chemical Imaging at the Nanoscale.

Publications: The first results were presented in an invited talk at Microscopy and Microanalysis 2005 and the Australian Conference on Microscopy and Microanalysis 2006.